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Crystallographic report

$Bi(S_2CNC_5H_{10})_2(NO_3)$(1,10-phenanthroline)

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The structure of $Bi(S_2CNC_5H_{10})_2(NO_3)$(1,10-Phen) features an eight-coordinated distorted square antiprismatic geometry around bismuth, defined by an $N_2O_2S_4$ donor set, with Bi–S distances ranging from 2.641(2) to 2.824(2) Å. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; bismuth complex; pyrrolinedithiocarbamate

COMMENT

The structural chemistry of bismuth complexes with dithiocarbamate ligands is rich and diverse. Thus, bismuth dithiocarbamate structures range from mononuclear,[1] to dimeric,[2,3] to linear polymeric.[4–6] In $Bi(S_2CNC_5H_{10})_2(NO_3)$(1,10-phen), Fig. 1, an eight-coordinated distorted square antiprismatic geometry around bismuth is found. The coordination geometry is defined by an $N_2O_2S_4$ donor set, with Bi–S distances ranging from 2.641(2) to 2.824(2) Å.

EXPERIMENTAL

An aqueous solution of $Bi(NO_3)_3 \cdot 5H_2O$ (1.0 mmol) and mannite (1.0 mmol) were added to an aqueous solution of sodium pyrrolinedithiocarbamate (2.0 mmol) and 1,10-phenanthroline (1.0 mmol), and stirred for 0.5 h at 30 °C. A yellow solid was recrystallized from an acetonitrile solution of the compound to give yellow crystals, m.p. 251 °C (dec.). Intensity data were collected at 298 K on a Bruker Smart 1000 CCD for a yellow block $0.07 \times 0.13 \times 0.15$ mm^3. $C_{24}H_{28}BiN_5O_3S_4$, $M = 771.73$, triclinic, $P\bar{1}$, $a = 10.358(3)$, $b = 11.304(4)$, $c = 13.911(5)$ Å, $\alpha = 97.915(5)$, $\beta = 95.682(5)$, $\gamma = 116.490(5)°$, $V = 1420.1(8)$ Å^3, $Z = 2$, 4877 unique data ($\theta_{max} = 25.0°$), $R = 0.085$ (all data), $wR = 0.058$. Program used: SHELXL and ORTEP. CCDC deposition number: 2201122.

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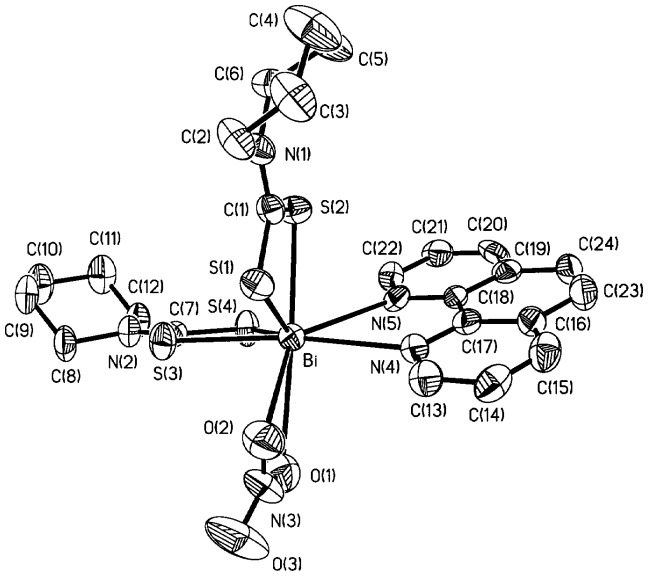

Figure 1. The molecular structure of $Bi(S_2CNC_5H_{10})_2(NO_3)$(1,10-Phen); hydrogen atoms have been omitted for clarity. Key geometric parametric parameters: Bi–S1 2.752(2), Bi–S2 2.641(2), Bi–S3 2.699(2), Bi–S4 2.824(2), Bi–O1 2.827(7), Bi–O2 2.845(7), Bi–N4 2.713(6), Bi–N5 2.794(5) Å; S1–Bi–S2, 66.0(2), S1–Bi–S3, 82.0(1), S1–Bi–S4 136.7(1), S1–Bi–O1 110.4(1), S1–Bi–O2 67.3(2), S1–Bi–N4 83.9(1), S1–Bi–N5 122.8(1), S2–Bi–S3 93.2(1), S2–Bi–O1 176.1(1), S2–Bi–O2 133.3(2), S2–Bi–S4 88.9(1), S2–Bi–N4 92.8(1), S2–Bi–N5 73.0(1), S3–Bi–S4 64.0(1), S3–Bi–O1 84.5(1), S3–Bi–O2 81.8(1), S3–Bi–N4 160.9(2), S3–Bi–N5 139.5(1), S4–Bi–O1 92.9(1), S4–Bi–O2 127.8(1), S4–Bi–N4 134.3(1), S4–Bi–N5 77.5(1), O1–Bi–O2 43.3(2), O1–Bi–N4 88.4(2), O1–Bi–N5 110.8(2), O2–Bi–N4 80.9(2), O2–Bi–N5 135.3(2), N4–Bi–N5 59.6(2)°.

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